

Machine Learning for Materials Hard and Soft

ESI-DCAFM-TACO_VDSP Summer School 2022

Schedule – Week 1

	Mon, 11 Jul	Tue, 12 Jul	Wed, 13 Jul	Thu, 14 Jul		Fri, 15 Jul
09.00	“Mathematical Introduction I” Philipp Grohs University of Vienna	“Mathematical Introduction II” Philipp Grohs University of Vienna	“Image Analysis” Thomas Pock TU Graz	“ML for electronic structure” James Spencer & David Pfau Deep Mind	09.00	Bingqing Cheng Institute of Science and Technology Austria (ISTA)
					09:45	Andrew Ferguson University of Chicago
10.30	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	10.30	<i>Coffee Break</i>
11.00	“Mathematical Introduction I” Philipp Grohs University of Vienna	“Mathematical Introduction II” Philipp Grohs University of Vienna	“Image Analysis” Thomas Pock TU Graz	“ML for electronic structure” James Spencer & David Pfau Deep Mind	11.00	Marjolein Dijkstra University of Utrecht
					11.45	“AI Case Studies” Marine Pigneur (MLR GmbH) Christopher Lepenik (Image Biopsy Lab) Christian Leitold (Verbund) Bhuiyan S.M. Ebna-Hai (Fehrmann)
12.30	<i>Lunch Break</i>	<i>Lunch Break</i>	<i>Lunch Break</i>	<i>Lunch Break</i>	12.45	<i>AI Lunch</i>
14.00 – 17.00	Tutorial Philipp Grohs University of Vienna	Tutorial Philipp Grohs University of Vienna	Tutorial Thomas Pock TU Graz	Tutorial James Spencer & David Pfau Deep Mind	14.30	Milica Todorovic University of Turku
					15.15	Reinhard Maurer University of Warwick
17.00	<i>Welcome reception</i>				16.00	Roberto Covino Frankfurt Institute for Advanced Studies (FIAS)

Registration: Monday, 11 July 2022, at 08.30 in front of ESI Boltzmann lecture hall, top floor, ESI, Boltzmanngasse 9a, 1090 Vienna

Lectures: ESI Boltzmann lecture hall | **Tutorials:** ESI Boltzmann & ESI Schrödinger lecture halls | **Coffee Break:** ESI common room | **Lunch Break:** self-organized

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Schedule – Week 2

	Mon, 18 Jul	Tue, 19 Jul	Wed, 20 Jul	Thu, 21 Jul	Fri, 22 Jul
09.00	“ML potentials” Philipp Marquetand University of Vienna	“ML potentials” Philipp Marquetand University of Vienna	“Statistical Sampling” Peter Wirnsberger Deep Mind	“Free energies and enhanced sampling” Luigi Bonati ETH Zurich & IIT Genova	“Materials properties prediction” Taylor D. Sparks University of Utah
10.30	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>
11.00	“ML potentials” Philipp Marquetand University of Vienna	“ML potentials” Philipp Marquetand University of Vienna	“Statistical Sampling” Peter Wirnsberger Deep Mind	“Free energies and enhanced sampling” Luigi Bonati ETH Zurich & IIT Genova	“Materials properties prediction” Taylor D. Sparks University of Utah
12.30	<i>Lunch Break</i>	<i>Lunch Break</i>	<i>Lunch Break</i>	<i>Lunch Break</i>	<i>Closing Remarks</i>
14.00 – 17.00	Tutorial Philipp Marquetand University of Vienna	Tutorial Philipp Marquetand University of Vienna	Tutorial Peter Wirnsberger Deep Mind	Tutorial Luigi Bonati ETH Zurich & IIT Genova	
18.00		<i>Social Dinner</i>			

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Lectures: ESI Boltzmann lecture hall | **Tutorials:** ESI Boltzmann & ESI Schrödinger lecture halls | **Coffee Break:** ESI common room | **Lunch Break:** self-organized